Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

First-Principles Studies of Octacyclopropylcubane: A Novel High-Energy Density Material[1] STEVEN L. RICHARDSON, Howard University, REESHEMAH N. ALLEN, DANIEL FINKENSTADT, Naval Research Laboratory, MICHAEL J. MEHL, MARK R. PEDERSON, Naval Research Laboratory
— The ongoing quest for synthesizing novel high-energy density materials (HEDMs) is clearly motivated by a search for new propellants and explosives. Recently de Meijere *et al.* have synthesized a new HEDM, octacyclopropylcubane ($C_{32}H_{40}$), in which the eight hydrogen atoms of cubane were replaced by cyclopropyl groups. In this work we report the results of a first-principles density-functional theory (DFT) calculation using the suite of codes known as NRLMOL (Naval Research Laboratory Molecular Orbital Library) to compute the structural, electronic, and vibrational properties of octacyclopropylcubane. We have calculated the vibrational properties of $C_{32}H_{40}$ and compare our results with experiment. We have also employed a DFT-based tight-binding scheme to compute the vibrational density of states for octacyclopropylcubane and compare our results with our full DFT-based results. Interesting enough, the geometry of the cyclopropyl groups in $C_{32}H_{40}$ does not allow for the quartic- concerted torsional mode (QCTM) that we and other workers have previously studied in octanitrocubane.

[1]We are grateful to ONR and NSF for financial support of this research.

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Date submitted: 21 Nov 2008 Electronic form version 1.4